Bayesian networks in environmental modelling

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Abstract

Bayesian networks (BNs), also known as Bayesian belief networks or Bayes nets, are a kind of probabilistic graphical model that has become very popular to practitioners mainly due to the powerful probability theory involved, which makes them able to deal with a wide range of problems.The goal of this review is to show how BNs are being used in environmental modelling. We are interested in the application of BNs, from January 1990 to December 2010, in the areas of the ISI Web of Knowledge related to Environmental Sciences. It is noted that only the 4.2% of the papers have been published under this item. The different steps that configure modelling via BNs have been revised: aim of the model, data preprocessing, model learning, validation and software. Our literature review indicates that BNs have barely been used for Environmental Science and their potential is, as yet, largely unexploited.

Keywords: Bayesian networks, Environment, Model implementation, Software, Review

1. Introduction

1.1. Methodological development of Bayesian networks

The term Bayesian network was first stated by Judea Pearl in 1986 (Pearl, 1986a), who formally characterized their expressive power and designed an

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algorithm for efficiently computing probabilities from a BN, but only for some particular network structures. But it was early in the 90s when BNs became really popular tools for dealing with uncertain domains, mainly due to the formulation of efficient algorithms for computing probabilities from BNs without structural restrictions (Jensen et al., 1990a; Shenoy and Shafer, 1990) and the release of the first software for modelling using BNs (Andersen et al., 1990).

The next step forward was the development of machine learning techniques for BNs, which dramatically expanded the potential applications of these models, giving the possibility of automatically inducing BNs from databases (Cooper and Herskovitz, 1992; Spirtes et al., 1993).

Later on, Friedman et al. (1997) promoted the use of BNs as tools for pattern recognition or classification, showing that these models were able to compete with well known classifiers, such as classification trees (Quinlan, 1986).

Another important advancement came along with the introduction of hybrid models, in which continuous and discrete variables were allowed to coexist. The first attempt was the so-called Conditional Gaussian model (Lauritzen, 1992), but it had the limitation of imposing structural restrictions to the possible networks. A more general framework is the one based on Mixtures of Truncated Exponentials (MTEs) (Moral et al., 2001) in which no structural restrictions are imposed.

Taking advantage of the possibility to handle continuous domains, BNs have recently been applied with remarkable success to regression problems (Fernández et al., 2007; Morales et al., 2007; Fernández and Salmerón, 2008; Fernández et al., 2010), in which the goal is to predict the values of a continuous response variable given the values of some explanatory variables.

1.2. Bayesian network definition

A Bayesian network (Jensen and Nielsen, 2007) is a statistical multivariate model for a set of variables $\mathbf{X} = \{X_1, \ldots, X_n\}$, which is defined in terms of two components:

- Qualitative component: A directed acyclic graph (DAG) where each vertex represents one of the variables in the model, and so that the presence of an edge linking two variables indicates the existence of statistical dependence between them.
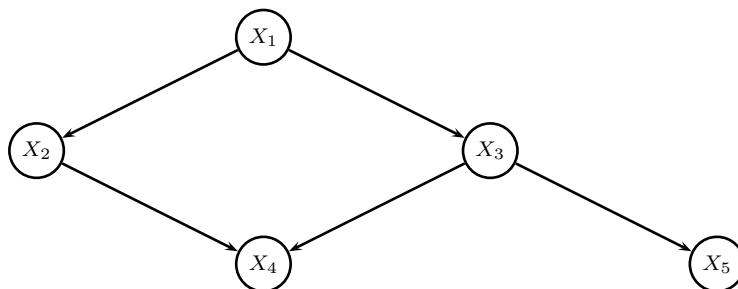
Figure 1: A Bayesian network with five variables.

- Quantitative component: A conditional distribution $p(x_i|pa(x_i))$ for each variable X_i, $i = 1, \ldots, n$ given its parents in the graph, denoted as $pa(x_i)$.

For example, the graph depicted in Figure 1 could be the qualitative component of a Bayesian network for variables $X_1, \ldots, X_5$. According to the structure of the graph, it would be necessary to specify a conditional distribution for each variable given its parents. In this case, the distributions are $p(x_1)$, $p(x_2|x_1)$, $p(x_3|x_1)$, $p(x_4|x_2, x_3)$ and $p(x_5|x_3)$.

1.2.1. Qualitative component of a Bayesian network

One of the most important advantages of Bayesian networks is that the structure of the associated DAG determines the dependence and independence relationships among the variables, so that it is possible to find out, with no need of carrying out any numerical calculations, which variables are relevant or irrelevant for some other variable of interest.

We will use a toy example from Jensen (2001) to explain the transmission of information in a Bayesian network.

Example 1.1 (Burglary or earthquake). *Mr. Holmes is working in his office when he receives a phone call from his neighbor Dr. Watson, who tells him that Holmes' burglar alarm has gone off. Convinced that a burglar has broken into his house, Holmes rushes to his car and heads for home. On his way, he listens to the radio, and in the news it is reported that there has been a small earthquake in the area. Knowing that earthquakes have a tendency to turn burglar alarms on, he returns to his work.*
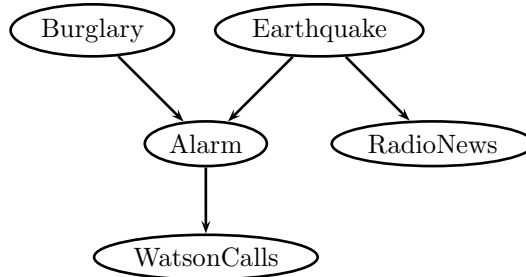
Figure 2: The Bayesian network for the *burglary or earthquake* example.

The scenario described in Example 1.1 can be represented by the Bayesian network in Figure 2. In general, there are only three types of connections among variables in a DAG: serial, converging and diverging connections. Therefore, it is enough to explain how information flows for these three types of connections. We will use the example above to illustrate this.

1. Serial connections. "Burglary" has a causal influence on "Alarm", which in turn has a causal influence on "Watson calls". Therefore, information flows from "Burglary" to "Watson calls" and vice versa, since knowledge about one of the variable provides information about the other. However, if we observe "Alarm", any information about the state of "Burglary" is irrelevant to our belief about "Watson calls" and vice versa, since once we have certainty about the fact that the alarm has gone off, the information provided by Watson does not change our state of belief.

2. Diverging connections. "Earthquake" has a causal influence on both "Alarm" and "Radio news". Therefore, information flows from "Alarm" to "Radio news" and vice versa, since knowledge about one of the variable provides information about the other. For instance, if our only knowledge is that the radio news reported a small earthquake, our belief about the alarm going off would increase. On the other hand, if we observe "Earthquake", i.e. we have certainty about that, any information about the state of "Alarm" is irrelevant for our belief about an earthquake report in the "Radio news" and vice versa.

3. Converging connections. "Alarm" is causally influenced by both "Burglary" and "Earthquake". However, in this case the last two variables are irrelevant to each other: if we do not have any information about the alarm, there is no relationship between the other two variables. However, if we observe "Alarm" and "Burglary", then this will effect our belief about "Earthquake": burglary explains the alarm, reducing our belief that earthquake is the triggering factor, and vice versa.

In general, applying these three rules, it is possible to determine the variables that are relevant to our goal variable.

1.2.2. Quantitative component of a Bayesian network

Once the structure is defined, it is necessary to know how strong the relationships are among the variables. This is achieved by using the quantitative component of the Bayesian network.

Taking into account the independencies encoded by the network structure, it holds that the joint distribution over all the variables is equal to the product of the conditional distributions attached to each node, so that

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i | pa(x_i)) \quad \forall x_1, \ldots, x_n \in \Omega_{X_1, \ldots, X_n}, \qquad (1)$$

in which Ω_{X_i} represents the set of all possible values of variable X_i.

Assume X_i is a variable in which we are interested, and X_E is a set of variables whose values can be known. Then, the prediction for the value of X_i given X_E can be obtained by computing the probability of each possible value of X_i given each possible configuration of X_E. This probability distribution can be obtained from the joint distribution in Equation (1). In fact, there is no need to compute the joint distribution, since there are efficient algorithms that allow the calculation of $p(x_i | x_E)$ taking advantage of the factorisation of the joint distribution imposed by the network structure (Shenoy and Shafer, 1990; Madsen and Jensen, 1999).

1.3. Pros and cons of Bayesian networks

Some pros of BNs in environmental modelling are:

(1) Since nodes are modelled by means of probability distributions, risk and uncertainty can be estimated more accurately than in models where

only mean values are taken into account (Uusitalo, 2007). This probabilistic representation makes BNs an appropiate tool for modelling environmental systems, since it can deal with uncertainty (Rieman et al., 2001; Ghabayen et al., 2004; McCann et al., 2006; Henriksen and Barlebo, 2008; Malakmohammadi et al., 2009; Wang et al., 2009; Haapasaari and Karjalainen, 2010).

(2) Since numeric values are attached to the relationship between the variables, the probability of a particular hypothesis can be automaticaly computed (Ordóñez-Galán et al., 2009).

(3) Once the model is learned, the probability distribution of a node given its parents is obtained, and even the other way round, the probability distribution of a parent node given its child nodes can also be obtained (Wooldridge and Done, 2004; Uusitalo, 2007), which allows us to know the effects given the causes and the causes given the effects (Getoor et al., 2004), and so they are used as inferential models (Nadkarni and Shenoy, 2004; Malakmohammadi et al., 2009).

(4) In environmental sciences, experts and stakeholders opinions are useful when modelling a problem/system, since they can guide the model to focus on the most important parts, or by evaluating the candidate model to find inconsistencies or differences with respect to established theoretical properties (Batchelor and Cain, 1999; Cain et al., 2003; McDowell et al., 2009; Wang et al., 2009; Cyr et al., 2010; Haapasaari and Karjalainen, 2010). However this procedure has to be done properly in order to avoid errors or bias in the model (Welp et al., 2006). BNs are able to incorporate expert knowledge via a participatory modelling procedure, since the relations between the variables can be visualized easily through the graphical representation of the network, and so they can be modified by the experts or stakeholders just by adding or removing variables and links in the graph (Voinov and Bousquet, 2010). This advantage makes them also easier to understand and visualize by the final users (Seroussi and Golmard, 1994; Bacon et al., 2002; Cain et al., 2003; Lacave et al., 2006; McCann et al., 2006; Henriksen et al., 2007; McDowell et al., 2009).

(5) BNs are able to model complex systems with a large number of variables (Getoor et al., 2004), in a quick and efficient way under some circum-

stances (Luo et al., 2005). If an exact solution is unreachable, there are algorithms available that can deliver an approximate solution, using simulation techniques or deterministic approximation methods (Cano et al., 2004).

(6) BNs are able to manage missing values in input data and perform the proper predictions with the model built from them (Woody and Brown, 2003; Nadkarni and Shenoy, 2004; Ozbay and Noyan, 2006; Uusitalo, 2007; Axelson et al., 2009; Bressan et al., 2009).

However, some authors also mention some limitations:

(1) The building process of the network and the parameter estimation requires more data as the number of variables increases (Pradhan et al., 1996; Tremblay et al., 2004; Ordóñez-Galán et al., 2009) as long as the accuracy in the estimations and in the network topology is to be maintained.

(2) The main problem is due to the fact that most of the data available are continuous or hybrid, and even though BNs can manage them, the limitations are too restrictive (Lauritzen, 1992; Nyberg et al., 2006; Uusitalo, 2007). The most extended solution is to discretize the variables, although some new solutions have been proposed, such as the Mixtures of Truncated Exponentials model (MTE) (Moral et al., 2001) or the Mixtures of Polynomials model (MP) (Shenoy and West, 2011), however these solutions are not yet available in the usual commercial BN software.

(3) Time series can be modelled as Dynamic BNs (Kjærulff, 1992; Jensen and Nielsen, 2007), since the links in the networks may be considered as the effect of time over the variables. However their complexity makes medium size models usually intractable, since the number of variables involved is greater than in static models (McCann et al., 2006; Zorrilla et al., 2010).

(4) Fuzzy models (Zadeh, 1965; Walley, 1991) are a different way to express ambiguity in a model, more related to imprecision or fuzzy events. BNs are useful tools to deal with probabilistic theory, but they are also able to handle these fuzzy models, using for example Credal networks (Cozman, 2000), in which the relation between two variables is expressed in

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terms of sets of probability distributions. However, these models are not yet incorporated to the usual commercial BN software, and so they are not available to the general scientific community.

2. Overview

A keyword search of the ISI web of Knowledge, for the period January 1990 to December 2010, using the search terms "Bayesian Networks", "Bayesian Belief Networks" and "Bayes Nets" was carried out. The topics selected were papers or reviews, resulting in 1375 documents retrieved. Figure 3 shows the distribution of papers by year of publication. Two phases can be identified: between 1990 and 2002 the number of papers published per year was less than 50; but from 2003 there was an exponential trend in the number of papers published, with 226 in 2010 alone.
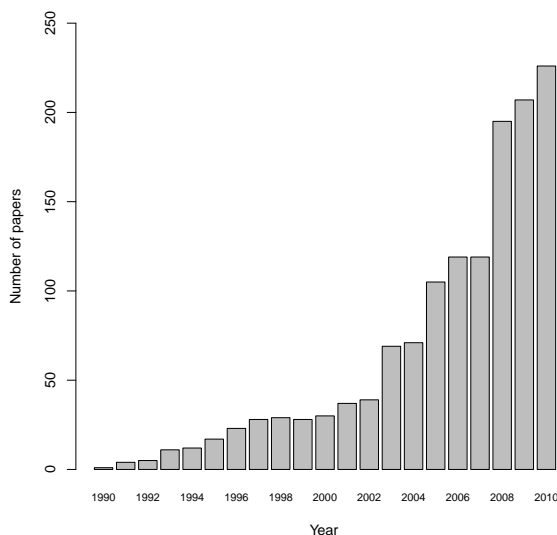

Figure 3: Bayesian networks publications in the last two decades.

Over the period reviewed, the highest proportion of publications relating to BNs fall into two subject areas (Computer Sciences and Mathematics; Table 1), while Environmental Sciences papers were infrequent (4.2%). These

Scientific area	Percentage
Computer Sciences	27.3
Mathematics	20.9
Engineering	16.2
Health Sciences	15.0
Life Sciences	10.9
Sociology and Education	4.4
Environmental Sciences	4.2
Others	1.0

Table 1: Percentage of papers in different scientific areas obtained from joining similar ISI Web of Knowledge subject areas. Others refer to Goverment Law, Public Administration, and Demography and Acoustics.

data indicate that, despite their potential, BNs have barely been applied in Environmental Sciences.

The review of papers related to environmental sciences, using the search terms "Bayesian Networks", "Bayesian Belief Networks" and "Bayes Nets" were achieved from the subjects areas: Environmental Sciences & Ecology, Agriculture, Water Resources, Marine & Freshwater Biology, Biodiversity & Conservation, Forestry, Geology, Meteorology & Atmospheric Sciences, Fisheries, Developmental Biology, Virology, Geography, Antrophology, Geochemistry & Geophysics, Demography, Zoology, Plant Sciences, Energy & Fuels, Evolutionary Biology, Mycology, Chemistry, Microbiology, Life Sciences & Biomedicine-Other Topics and Operations Research & Management Science. We only obtained valid references from the first nine subject areas mentioned above. The list obtained was refined to exclude papers not related to Environmental Sciences or Bayesian networks. The search was extended manually to papers and journals outside the scope of the ISI Web of Knowledge. Finally 128 papers were selected. In Table 2 these papers are classified according to the different ISI Web of Knowledge subject areas. Those papers assigned by the ISI Web of Knowledge to more than one subject area and those from journals not included in the index were assigned to a specific subject area according to our criteria. From the total of 128 papers selected, 14 do not build any BN model, despite they discuss about BNs and Environmental Sciences. These papers are assigned to a general category named

"Others".

Table 3 lists the different features of a BN, thoroughly explained in Section 3, and Table 4 shows the results of the papers reviewed.

3. Model implementation

The process of modelling involves different steps (Marcot et al., 2006; Nyberg et al., 2006; Maier et al., 2010). A general procedure applicable to the BN modelling can be summarized as follows:

1. Identification of the aim of the model.
2. Data pre-processing: Data preparation and refinement.
3. Model learning: Build the model from available information.
4. Validation: Check the representativity of the model and the accuracy of the inference results.

Each of these steps can be done is many different ways. This is what will be explained in the remainder of this section.

3.1. Aim of the model

The first result we obtain when modelling a problem through a BN is a characterization of the actual problem, in terms of the relationships between the different variables and their strength. Due to the (in)dependence relationships expressed in the graph through the presence or absence of links, this information is presented in a clear and simple way.

One of the most interesting features of BNs is their ability to compute posterior probabilities, given some evidence. We call *evidence or finding* the knowledge about the value of one or more variables of the model. The computation of the posterior probability is called inference, evidence propagation or belief updating. It is an interesting tool since we can observe the change, in terms of probability, of some variables, given the value of some others. A lot of different algorithms to compute probabilities have been proposed by different researchers. Exact algorithms are usually based on the idea of performing the computations locally, e.g., the fusion algorithm (Pearl, 1986b, 1988), the variable elimination method (Zhang and Poole, 1996) and the junction tree algorithm (Lauritzen and Spiegelhalter, 1988; Jensen et al., 1990a,b). Although the independence relationships may help, computing probabilities in a BN can be too costly (Cooper, 1990); to solve partially

Category	#	References
Environmental Science & Ecology (ES&E)	37	Aalders and Aitkenhead (2006), Aitkenhead and Aalders (2009), Bacon et al. (2002), Borsuk et al. (2004), Dlamini (2010), Dorner et al. (2007), Faisal et al. (2010), Farmani et al. (2009), Fernandes et al. (2010), Haapasaari and Karjalainen (2010), Hosack et al. (2008), Howes et al. (2010), Johnson et al. (2010a), Kocabas and Dragicevic (2009), Lehmkuhl et al. (2001), Liedloff and Smith (2010), Little et al. (2004), Lynam et al. (2010), Marcot et al. (2001), Mesbah et al. (2009), Milns et al. (2010), Molina et al. (2009a), Nash et al. (2010), Newton (2010), Pal et al. (2001), Park and Stenstrom (2008), Pellikka et al. (2005), Pollino et al. (2007b), Qu et al. (2008), Raphael et al. (2001), Steventon et al. (2006), Steventon and Daust (2009), Stiber et al. (1999), Ticehurst et al. (2007), Varis and Kuikka (1997b), Voie et al. (2010), Walshe and Massenbauer (2008)
Water Resources (WR)	30	Ames et al. (2005), Barton et al. (2008), Batchelor and Cain (1999), Borsuk et al. (2001), Bromley et al. (2005), Calder et al. (2008), Castelletti and Soncini-Sessa (2007b), Chan et al. (2010), Cheon et al. (2008), Dawsey et al. (2006), Ghabayen et al. (2004), Henriksen et al. (2007), Henriksen and Barlebo (2008), Kollat et al. (2008), Kragt et al. (2010), Malakmohammadi et al. (2009), Martínez-Santos et al. (2010), Molina et al. (2009b), Park and Stenstrom (2006), Robertson et al. (2009b), Robertson et al. (2009a), Said et al. (2005), Said (2006), Santa Olalla et al. (2005), Santa Olalla et al. (2007), Saravanan (2008), Stow et al. (2003), Varis and Keskinen (2006), Wang et al. (2009), Zorrilla et al. (2010)
Agriculture (A)	9	Bashari et al. (2009), Bressan et al. (2009), Cain et al. (2003), Gambelli and Bruschi (2010), Holt et al. (2006), Kristensen and Rasmussen (2002), McDowell et al. (2009), Saravanan (2010), Tari (1996)
Geology (G)	7	Eidsvik et al. (2004), Grêt-Regamey and Straub (2006), Hapke and Plant (2010), Harris et al. (2009), Oliveros et al. (2008), Porwal et al. (2006), Qin et al. (2006)
Marine & Freshwater Biology (MF&B)	9	Grech and Coles (2010), Langmead et al. (2009), Reinert and Peterson (2008), Renken and Mumby (2009), Shenton et al. (2010), Stelzenmüller et al. (2010), Stewart-Koster et al. (2010), Ticehurst (2008), Wooldridge and Done (2004)
Biodiversity & Conservation (B&C)	8	Aguilera et al. (2010), Johnson et al. (2010b), McNay et al. (2006), Newton et al. (2007), Pollino et al. (2007a), Smith et al. (2007), Tattari et al. (2003), Wilson et al. (2008)
Forestry (Fo)	6	Cyr et al. (2010), Henderson and Burn (2004), Ordóñez-Galán et al. (2009), Rieman et al. (2001), Stassopoulou et al. (1998), Walton and Meidinger (2006)
Fisheries (Fi)	5	Axelson et al. (2009), Giles (2008), Haapasaari et al. (2007), Hammond and O'Brien (2001), Uusitalo et al. (2005)
Meteorology and Atmospheric Sciences (M&AS)	3	Barrientos and Vargas (1998) , Mount and Stott (2008), Varis and Kuikka (1997a)
Others	14	Aspinall et al. (2006), Castelletti and Soncini-Sessa (2007a), Croke et al. (2007), Hammond (2004), Lynam et al. (2007), Marcot et al. (2006), McCann et al. (2006), Nyberg et al. (2006), Pshenichny et al. (2009), Ricci et al. (2003), Tremblay et al. (2004), Uusitalo (2007), Varis (1997), Varis and Kuikka (1999)
TOTAL	**128**	

Table 2: Papers reviewed by subject.

Characteristic	Options	Abbreviations
	Inference	I
	Characterize	C
Aim of the model (A)	Classification with fixed str.	Clf
	Classification (no str.)	Clg
	Regression	R
	Discrete	D
	Discretize	Dis
Variable (Var)	Continuous	C
	Hybrid	Hy
	No information	NI
	Experts	Exp
	Software	Soft
	Equal Frecuency Interval	EFI
Discretize (Dis)	Entropy minimizator	EM
	Deterministic equations	DE
	Several	S
	No information	NI
	Data	D
Model learning (ML)	Experts	Exp
	Both	B
	No information	NI
	Train & Test	TT
	Cross Validation	CV
	Experts	Exp
	Previous models	Pm
Validation (Val)	Sensitivity analysis	SA
	Goodness of fit	Gof
	Several	S
	No validation	NV
	Analytica	A
	WINBUGS	W
	B-course	Bc
	Elvira	E
	C++	C
	Genie	G
Software (Soft)	Hugin	H
	Netica	N
	SamIam	SA
	Matlab	M
	Weka	We
	Several	S
	No information	NI

Table 3: Abbreviations for each option of the characteristics under study. Experts refer to domain experts, stakeholders and/or literature.

Char.	opt.	ES&E	WR	A	G	M&FB	B&C	Fo	Fi	M&AS	Total	%
A	I	28	24	8	3	5	4	3	4	2	81	71.1
	C	1	2	0	1	1	1	0	0	0	6	5.3
	Clg	7	1	0	2	3	2	3	1	1	20	17.5
	Clf	1	2	1	1	0	1	0	0	0	6	5.3
	R	0	1	0	0	0	0	0	0	0	1	0.9
Var	D	20	13	6	3	6	4	5	2	1	60	52.6
	Dis	9	13	3	2	2	1	1	3	1	35	30.7
	C	3	1	0	0	0	1	0	0	0	5	4.4
	Hy	0	1	0	0	0	1	0	0	0	2	1.8
	NI	5	2	0	2	1	1	0	0	1	12	10.5
Dis	Exp	1	3	2	0	0	1	1	1	0	9	25.7
	Soft	1	0	0	0	0	0	0	0	0	1	2.9
	EFI	0	1	0	0	0	0	0	0	0	1	2.9
	EM	0	0	0	1	0	0	0	0	0	1	2.9
	DE	0	3	0	0	0	0	0	0	0	3	8.6
	S	2	0	0	0	1	0	0	0	0	3	8.6
	NI	5	6	1	1	1	0	0	2	1	17	48.6
ML	D	9	4	0	2	1	1	0	0	1	18	15.8
	Exp	9	14	3	1	2	3	3	2	1	38	33.3
	B	17	9	6	3	5	4	3	2	1	50	43.9
	NI	2	3	0	1	1	0	0	1	0	8	7.0
Val	TT	3	3	0	1	0	1	2	0	0	10	8.8
	CV	3	1	1	2	1	1	1	0	0	10	8.8
	Exp	4	6	1	0	1	0	2	0	1	15	13.2
	Pm	2	0	0	0	0	0	0	1	0	3	2.6
	SA	5	4	2	1	2	0	1	0	0	15	13.2
	Gof	1	1	0	0	0	0	0	0	1	3	2.6
	S	5	4	1	0	2	3	0	0	0	15	13.2
	NV	14	11	4	3	3	3	0	4	1	43	37.7
Soft	A	1	1	0	0	0	0	0	0	0	2	1.8
	W	0	0	0	0	0	1	0	0	0	1	0.9
	Bc	0	0	0	1	0	0	0	0	0	1	0.9
	E	0	0	0	0	0	1	0	0	0	1	0.9
	G	0	0	1	0	0	0	0	0	0	1	0.9
	H	4	10	3	1	0	2	0	3	0	23	20.2
	N	15	7	2	1	6	3	3	2	0	39	34.2
	C	0	1	0	0	0	0	0	0	0	1	0.9
	SA	0	0	0	0	1	0	0	0	0	1	0.9
	M	1	0	0	0	0	0	0	0	0	1	0.9
	We	1	0	0	0	0	0	0	0	0	1	0.9
	S	3	1	0	0	0	0	1	0	0	5	4.4
	NI	12	10	3	4	2	1	2	0	3	37	32.5

Table 4: Number of papers analyzed in terms of the characteristics under study, its options, and subject areas.

this problem, some approximate algorithms have been proposed. These algorithms do not return the actual probability distribution of the variables of interest, but an approximation to it. Approximate algorithms can be divided into two different groups: methods based on simulation, that obtain a sample of the variables in the network via Monte Carlo simulation, and the marginal probability distributions are then estimated from it (Fung and Chang, 1990; Dagum and Luby, 1997; Hernández et al., 1996, 1998; Salmerón et al., 2000) and deterministic methods, based on different ideas, e.g., replace low-probability values by zeros, to decrease complexity, (Jensen and Andersen, 1990), or simplify the network structure removing weak dependencies (Kjærulff, 1994). These algorithms are implemented internally in the usual commercial BN software packages, and so the final user may not be aware of using them. That is the reason why most of the papers do not state the algorithms they use, and so we have not included this topic in the results of the review. The same happens with the algorithms about structural learning of the model, explained in Section 3.3.

A specific problem related to inference is *classification*. In a classification problem we are interested in predicting the value of one of the variables, usually denoted as class variable, given the values of some of the remaining variables, called feature variables. This is done via the inference process mentioned before. The main difference with respect to the above results is that our interest lies on one of the variables, and so we can concentrate and try to model as precisely as possible the relationships regarding the class variable, and not pay so much attention to the others. In fact, the BN is constructed in such a way that it is more feasible that it returns the correct value of the class variable given the evidence, rather than trying to accurately model the joint probability of all the variables in the network. Although any BN can be used for classification, in order to stress the importance of the class variable, some fixed-structure BN models are used, like the Naïve Bayes (Duda et al., 2001), Tree Augmented Network (Friedman et al., 1997) and kDB (Sahami, 1996) models.

If instead, our aim is to predict the value of a continuous target variable, then we are interested in a regression model. Regression models are widely known in the Statistics literature (Faraway, 2005), however, they can also be expressed as a BN (Fernández et al., 2007; Morales et al., 2007; Fernández and Salmerón, 2008; Fernández et al., 2010), with some advantages: we do not need to know the value of every variable to predict the value of the response variable, and a complete probability distribution is returned for the

target variable, so that the prediction values can be the mean value, mode, median, or some other central tendency measure. Figure 4 shows the results of the review process according to the different aims of the models.
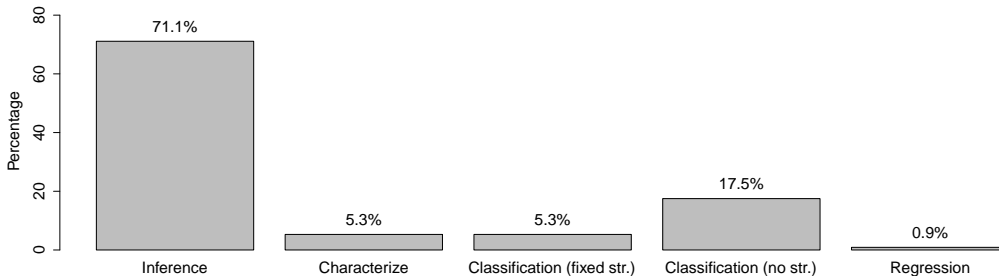

Figure 4: Aim of the model in the papers reviewed.

3.2. Data pre-processing

Before starting the process of learning, we have to prepare the data in such a way that learning algorithms can deal with them. Data pre-processing requires to address the following issues:

Type of variables: general BNs were initially implemented for discrete random variables. However, later on, some specific BN models were developed, incorporating the ability to deal with continuous or hybrid (discrete and continuous) domains (Lauritzen and Wermuth, 1989; Lauritzen, 1992; Cowell et al., 1999; Moral et al., 2001; Rumí et al., 2006; Langseth et al., 2009). These models impose some restrictions over the structure of the networks, as well as over the probability distributions. They are proved to perform better than discrete models, if the above mentioned restrictions are consistent with the problem under consideration, since no error approximation is introduced, but specific algorithms are needed to perform inference on them. If the use of some of these models is not possible, we need first to discretize the continuous values of our database, and then proceed as if all the variables were discrete. The discretization of a variable is the process of modifying its values so that it is transformed into a discrete one. There are several algorithms to do this, like entropy minimization, equal width and equal

frequency binning, deterministic equations, k-means, dynamic discretization (Dougherty et al., 1995; Kozlov and Koller, 1997; Christofides et al., 1999), but in general the result is an approximation to the actual data, which implies loss of information. The narrower the discretization band, the smaller the error that is added to the model. Figure 5 shows the percentage of the papers according to the type of variables, and Figure 6 shows the distribution of the different discretization methods found in the review process.
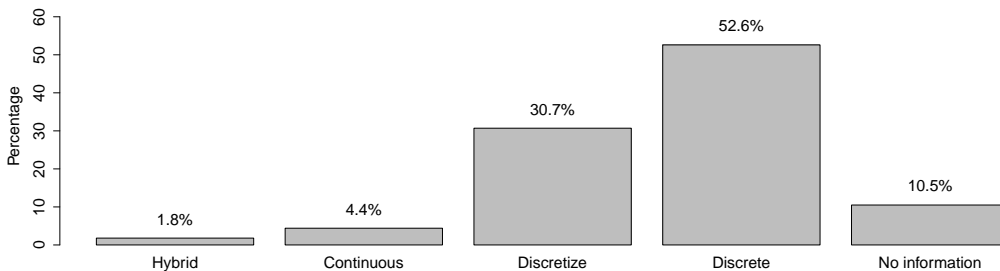
Figure 5: Type of variables in the papers reviewed. No information means the percentage of papers that gave no information about the type of the variables of the model.

Number of variables: nowadays it is easy to find extremely large databases (variables and cases). The presence of many cases in the database implies that the estimation of the distributions and the (in)dependence relationships will be recovered more precisely. However, increasing the number of variables in the network raises the complexity of the problem exponentially, and more data are needed to estimate the probability distributions properly. Some of the variables may represent the same information, so not every variable of the database has to be part of the BN model. In the articles reviewed, the number of variables ranged from 3 to 63, although 57.9% of the papers omit the number of variables employed.

Missing values: most of the classical statistical techniques are not able to deal with missing values. If only one value is missing in a case of the database, even though the rest of values are present, the entire case is dropped, with the corresponding loss of information. In contrast, learning algorithms of
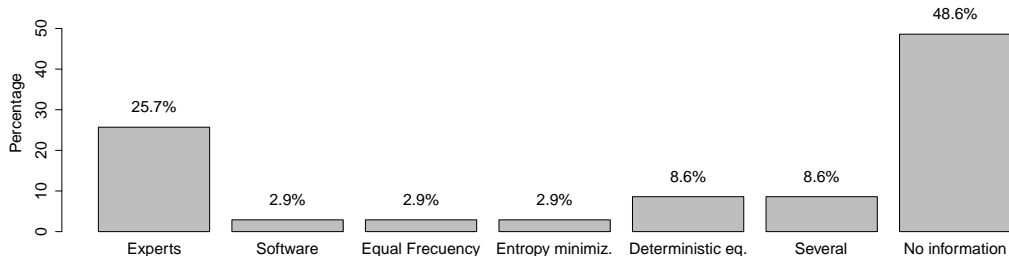
Figure 6: Discretization methods in the papers reviewed. Note that only papers that discretized the data are considered. No information means the percentage of papers that gave no information about how the discretization was carried out. Several makes reference to papers that apply different methods to different variables of the model. They include experts, equal frequency and equal width.

BNs can be adapted to use the Expectation Maximization algorithm (Dempster et al., 1977; Lauritzen, 1995) and benefit from the partial information contained in a case with missing values. This makes BNs excellent tools to deal with very expensive or corrupted data.

Our literature review highlighted that only 9.6% of the networks constructed worked with missing values.

3.3. Model learning

This is the main step when modelling a problem using BNs. As mentioned in Section 1, a BN has two main components, a qualitative component, i.e. the graph structure, and a quantitative component, the probability distributions. These two components have to be learned in connection, since the graph structure conditions the distributions to be estimated.

Once the graph structure is learned, the probability distributions are obtained by estimating the corresponding parameters; in the case of a general discrete BN, the parameters of a multinomial distribution are estimated by maximum likelihood, which is reduced to frequency counts, or a more sophisticated formula is applied, like the Laplace correction (Good, 1965), oriented to avoid zero-probabilities. In the case of continuous or hybrid BNs some

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other procedures are available (Castillo and Gutiérrez, 1998; Moral et al., 2003; Rumí et al., 2006; Langseth et al., 2010).

So, the structure selection defines the BN. As mentioned before, there are specific BN models with a fixed structure, e.g., Naïve Bayes and TAN, but general BNs require a procedure to select the structure from the information available.

Learning a structure implies discovering the (in)dependence relationships between the variables, so one of the methods in the literature is based on conditional independence tests, the so-called PC algorithm (Spirtes et al., 1993).

A BN can also be seen as an abstraction of the database, and so the problem can be reformulated as follows: "which is the BN among all possible BNs that best represents the database?" In this sense, structure learning is an optimization problem, where the solution is a BN in the set of all BNs. This is the approach of the K2 method (Cooper and Herskovitz, 1992) and similar ones (Romero et al., 2006). In order to check if one BN is better than another, we need a measure of how good a BN is. There are many of them, but one of the most frequently used is based on the Bayesian Information Criterion (BIC) measure (Schwarz, 1978), which depends on the likelihood and complexity of the estimated model.

Learning the structure of a BN directly from data may require a great amount of data, however, as mentioned in Section 1.3, one of the advantages of BNs is the possibility to incorporate expert knowledge to the model, in such a way that the network is fully defined by the experts, or they incorporate their knowledge to the network, for instance, by fixing a particular part of the graph, while learning the rest from data, or stating probabilities for particular events, considered as fundamental in the domain of application. Figure 7 shows the percentage of the papers depending on the learning procedure.

3.4. Validation methods

Depending on the aim of the model, the validation methods will be different. If the model was constructed to characterize or perform inference, the validation can be carried out through a different model which also represents the same problem, or via stakeholders, to assess the relationships expressed in the model. If the BN has a target variable, a sensitivity analysis (Jensen and Nielsen, 2007) is also useful to determine which variables and states of the variables are more influential with respect to the target variable. It shows
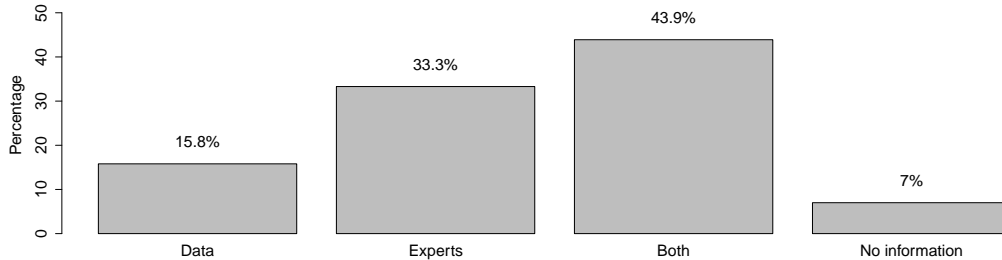
Figure 7: Model learning in the papers reviewed. Both makes reference to papers that combine expert knowledge and data. No information means the percentage of papers that do not state how the model was learned.

when small changes in the probability of a state returns great changes in the probability distribution of the target variable.

In the case of regression and classification scenarios, as any statistical tool, BNs are learned from a set of cases, but intended to perform properly for a wider range of data. To avoid the so-called overfitting, the database is split into two different sets, a bigger one used for training the model, called the training set and a smaller set called test set used to test the model. Then, some measure of the accuracy of the model performance is computed, e. g. log-likelihood, root mean squared error, prediction accuracy. The division is usually made randomly, selecting about 80% of the data for training and the rest for testing. If the same set of cases were used both for learning and testing, then obviously, the performance measure would be higher, but not so reliable. However, this train and test technique can produce a high variance of the validation measure. To avoid this, two techniques can be used: Cross validaton and Leave-one-out (Stone, 1974). These algorithms learn several models, using in each of them different sets of train and test sets, and the final performance measure is the average of the performances of all of them. In this way, every data case has been used both for training and testing the model, and since the different estimations of the validation measure are negatively correlated, the final variance of the estimated validation measure is decreased.

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It should be noted that, the estimated model should be learned with the entire data set, even though the validation method used is <u>Train & Test or Cross Validation.</u> The data division is only carried out in order to check the model, but not to develop a final model, especially if it is to be used in a final-user application. In that case the main interest is that the model behaves as accurately as possible, and this is achieved by using in the learning process as much information as possible.

An alternative validation method is carried out by means of a <u>Goodness of fit</u> procedure, in which the results obtained with the model are compared with the actual results from the database (real-world data), with no data division. Figure 8 shows the general distribution of the papers according to the validation method carried out, whilst Figures 9 and 10 show this distribution depending on the aim of the model.
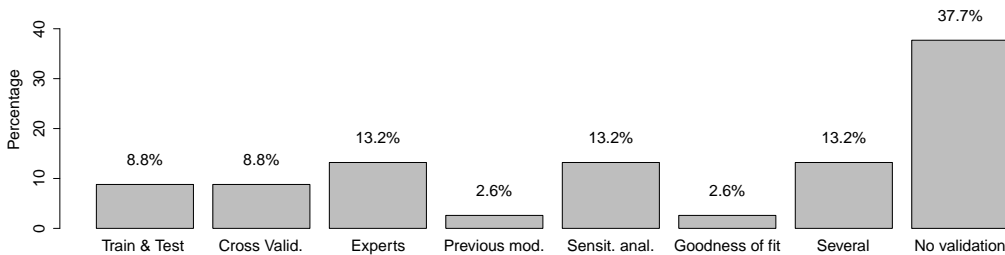
Figure 8: Validation methods in the papers reviewed. No validation means the percentage of papers that do not validate the model. Several makes reference to papers that apply different validation methods. They include experts, train & test, sensitivity analysis and prior models.

3.5. Software

As soon as the problem is medium-sized, the use of a computer and a proper software to learn the model and compute the distributions is necessary. Commercial and free software packages available are able to deal with many of the components of a BN model problem. In Korb and Nicholson (2003) and Murphy (2007) different software tools for managing BNs are explained
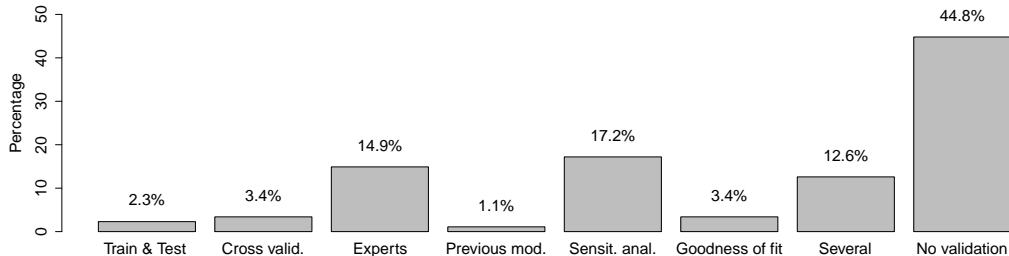
Figure 9: Validation methods when the aim of the model was characterization or inference in the papers reviewed. No validation means the percentage of papers that do not validate the model. Several makes reference to papers that apply different validation methods. They include experts, train & test, sensitivity analysis and prior models.

and compared. Figure 11 shows the results of the review process according to the software used.

4. Analysis of the results

In this section we highlight some of the results of the previous one: (1) Despite the great potential of BNs to perform classification or regression tasks, it should be emphasized that only 22.8% of the reviewed papers learn classification models, and only one paper solves a regression problem, while in 71.1% of the papers the aim of the model is inference. In particular, only 6 out of the 26 papers whose aim is classification use any of the well known classification-oriented graphical structures. (2) With respect to the type of variables, we can observe that 83.3% (including discrete and discretized variables) of the learnt models are discrete, in contrast to the 6.2% (including continuous and hybrid variables) of papers that directly handle continuous variables (3) Regarding validation methods, 37.7% of the reviewed papers do not validate the model, even though that percentage decreases to 14.8% for classification or regression models. (4) Expert knowledge is the most used method in the discretization (25.7%), model learning (77.2% including experts and both) and validation (13.2%) processes. However, in classification
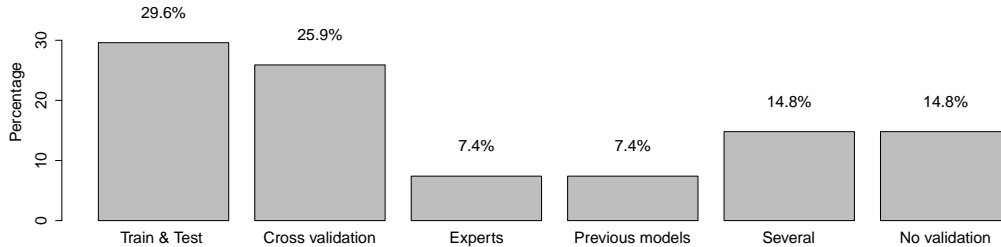
Figure 10: Validation methods when the aim of the model was classification or regression in the papers reviewed. No validation means the percentage of papers that do not validate the model. Several makes reference to papers that apply different validation methods. They include train & test and sensitivity analysis.

and regression models, validation through experts is the less used method (7.4%). (5) We have found lack of information in every step of the model implementation. Specially in the discretization methods (48.6%), validation methods (37.7%) and software used (32.5%).

5. Conclusions and recommendations

The literature review has highlighted how a large proportion of publications about BNs are from the fields of Mathematics and Computer Science. This suggests that most of the research effort has been put on the theoretical and methodological development, as well as on software implementation issues.

Looked at from another point of view, it is clear that, despite the existence of commercial software, use of BNs in Environmental Sciences is still scarce. In environmental studies, BNs are mainly applied as a technique for inference, using discrete data or discretized continuous variables. Environmental Science experts play a fundamental role in the training and validation of the models.

We think that the distribution of the papers shown in Table 4 is biased due to two different factors. First, the software used to learn and interact
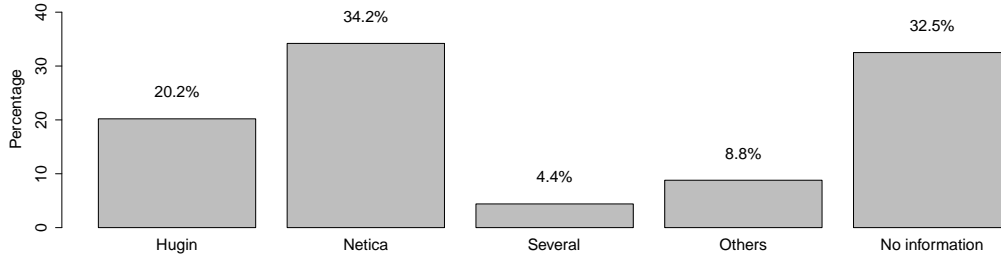
Figure 11: Software applied to configure the structure in the papers reviewed. Others makes reference to the software used at most in two papers. They include WinBugs, B-course, Elvira, GeNie, C++, Weka, Matlab and Analytica. Several makes reference to papers that use different software in the same paper. They include Netica, Matlab, Hugin, Microsoft Visual Basic, Microsoft Excel and GeNie & Smile. No information means the percentage of papers that do not indicate the software used.

with the model determines implicitly which procedures can be carried out and which ones cannot. Just to mention a few, hybrid BNs are not allowed in every software, and if so, in most of the cases the Conditional Gaussian model is the only solution apart from simulation or discretization. Following this argument, the validation of the model can only be done if the software includes this feature, as for example, Cross Validation. Second, the affiliation of the authors should also be taken into account; interdisciplinary works usually reflect both the computer science and the environmental sides in the paper, and so, the limitation of the software is in some sense overcome. Although these papers stress the environmental solution of the problem, the BN methodology carried out is clearly stated.

Based on this review we can make the following recommendations for future work:

(1) Though BNs were initially implemented for use with discrete data, some BN models are able to work with continuous or hybrid variables, avoiding the introduction of errors during the discretization phase. Therefore, a useful development would be the application of the algorithms

referenced in Section 1 that allow continuous and hybrid data to be processed in the same network environment.

(2) Environmental studies are sometimes obliged to work with missing values, which means that data cannot be processed using the traditional statistical techniques. We recommend the use of BNs in environmental studies with missing values, since BNs provide appropriate solutions for this problem.

(3) A high percentage of the studies using BNs did not validate the model. We suggest to the researchers to choose, from the many validation techniques available, the one that best fits the objective of the model.

(4) As mentioned in Section 1.3, BNs are a valid tool for Participatory environmental modelling with experts and stakeholders, due to the ease of interpretation and modification of the graph. This ease of modification may become a problem, if the experts and stakeholders are not aware of the concepts involved in the graphical representation of the BN expressed in Section 1.2.1. We recommend the use of methods for incorporating expert knowledge properly in a BN, as for example the proposed by Heckerman et al. (1995) and Cano et al. (2011).

(5) We observe that the studies reviewed do not use a common language for their BN modelling. There is a need for interdisciplinary meetings between scientists where the language of BN modelling can be standardized.

Acknowledgements

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